Amendments to the Claims:

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1. (Currently Amended). A method for calculating the similarity of at least one chemical compound to at least one chemical probe, ~~the at least one chemical probe including at least another chemical compound, the method~~ comprising the steps of:

(a) ~~creating~~ utilizing at least one chemical descriptor for each ~~compound in~~ of a ~~collection~~ plurality of compounds, each descriptor comprising a row of a molecule-descriptor matrix *X*;

(b) representing ~~at least one chemical descriptor for~~ each compound as ~~at least one~~ a column ~~vector comprising~~ of the ~~at least one~~ molecule-descriptor ~~frequencies~~ matrix, the entries of the molecule-descriptor matrix comprising a mathematical function of the weighting of each descriptor for each compound;

(c) ~~representing the collection of compound the at least one vector as a first vector of a molecule-descriptor matrix;~~

~~(d)~~ performing a singular value decomposition (SVD) of the molecule-descriptor matrix to produce ~~at least one singular matrix~~ resultant matrices;

~~(e)~~ (d) ~~generating at least one~~ creating a chemical probe descriptor vector for the at least one chemical probe, the entries of the chemical probe descriptor vector comprising a mathematical function of the weighting of each descriptor for each chemical probe;

~~(f)~~ (e) using ~~the~~ at least one ~~singular matrix~~ of the resultant matrices to ~~transform~~ calculate the ~~at least one chemical probe descriptor of the at least one chemical probe into a first coordinate system at least substantially similar to a second coordinate system of the at least one compound;~~ similarity between the at least one chemical probe and at least one compound of the molecule descriptor matrix; and

~~(g) calculating the similarity of transformed probes to the compounds in the collection, and~~

~~(h)~~ (f) ~~outputting a list of at least a subset of compounds in the collection ranked in order of~~ providing an output indicating the similarity ~~to~~ between the at least one chemical probe and the at least one ~~probe~~ compound.

2. (Currently Amended). The method as recited in claim 1, wherein ~~said step of creating~~ each of the at least one ~~descriptor includes generating~~ chemical descriptors comprise at least one of an atom pair descriptor and a topological torsion ~~descriptors from chemical connection tables of the collection of compounds~~ descriptor.

3. (Canceled).

4. (Currently Amended). The method as recited in claim 1, wherein said ~~molecule descriptor matrix is denoted as X, wherein said step of~~ performing ~~singular value decomposition includes~~ step comprises the steps of:

generating ~~singular~~ resultant matrices ~~as~~ $[[X = P\Sigma Q^T]]$ ~~of rank r~~ P, Σ and Q^T, such that molecule-descriptor matrix $X = P\Sigma Q^T$, wherein

P is a mxr matrix, called the left singular matrix (r is the rank of X), and its columns are the eigenvectors of XX^T corresponding to nonzero eigenvalues;

Q is a nxr matrix, called the right singular matrix, whose columns are the eigenvectors of X^TX corresponding to nonzero eigenvalues; and

Σ is a rxr diagonal matrix whose nonzero elements, $\sigma_1, \sigma_2, \ldots, \sigma_r$ called singular values, are the square roots of the eigenvalues and have the property that $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r$, ~~and~~

~~a reduced dimension approximation of X, defined as $X_k = P_k \Sigma_k Q^T_k$ k << r, where, P and Q are the left and right singular matrices representing correlations among descriptors and compounds respectively, and Σ represents the singular values,~~

~~wherein the at least one produced singular matrix includes a pseudo-object denoted as O_F and is calculated from a probe F by $O_F = F^T P_k \Sigma^{-1}_k$, and~~

~~wherein said step of calculating the similarity between the pseudo-object O_F and the compounds in collection is computed by taking a dot product of a normalized vector of O_F, with each normalized row of~~ [[P_k]].

5. (Currently Amended). The method as recited to claim 4, wherein said similarity ~~calculating step includes calculating cosine between each pair of vectors~~ between the at least one chemical probe and at least one compound of the molecule descriptor matrix is computed in accordance with the following steps:

generating a reduced dimension approximation of X, defined as $X_k = P_k \Sigma_k Q^T_k$, $k < r$;

generating a pseudo-object, denoted as O_F, where $O_F = F^T P_k \Sigma^{-1}_k$, and where F is a molecule-descriptor vector for the at least one chemical probe; and

taking a dot product of O_F with one or more columns of Q^T_k respectively corresponding to the at least one compound.

6. (Currently Amended). The method as recited in claim [4] 5, wherein ~~said step of performing singular value decomposition includes deriving the reduced dimensional approximation of X by setting the k+1 through r singular values of~~ [[Σ]] σ_{k+1} to σ_r are equal to zero for Σ_k.

7. (Currently Amended). The method as recited in claim [4] 5, wherein ~~similarities of the pseudo-object to compounds in the collection is calculated by setting the first k singular values of~~ [[Σ]] σ_1 to σ_k are equal to one for Σ_k.

8. (Currently Amended). The method as recited in claim 7, wherein Σ_k ~~said setting step includes using~~ comprises an identity matrix I.

9. – 21. (Canceled).

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22. (New). The method according to claim 1, wherein in said representing step the weighting comprises a frequency.

23. (New). The method according to claim 22, wherein in said creating step the weighting comprises a frequency.

24. (New). The method according to claim 5, wherein X_k is the least squared closest to X.

25. (New). A method for calculating the similarity between two chemical descriptors represented in a molecule-descriptor matrix X, comprising the steps of:

(a) utilizing at least one chemical descriptor for each of a plurality of compounds, each descriptor comprising a row of the molecule-descriptor matrix X;

(b) representing each compound as a column of the molecule-descriptor matrix, the entries of the molecule-descriptor matrix comprising a mathematical function of the weighting of each descriptor for each compound;

(c) performing a partial singular value decomposition (SVD) of the molecule-descriptor matrix to produce resultant matrices P_k, Σ_k, and Q_k, such that partial matrix $X_k = P_k \Sigma_k Q^T{}_k$, is the least squares closest approximation of X for any given k, $k < r$, where r is the rank of the matrix X;

(d) calculating the similarity between two chemical descriptors i and j by computing the dot product between row i and row j of the matrix P_k; and

(e) providing an output indicating the similarity between the two descriptors.

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26. (New). A method for calculating the similarity of at least one chemical descriptor and at least one chemical probe, comprising the steps of:

(a) utilizing at least one chemical descriptor for each of a plurality of compounds, each descriptor comprising a row of a molecule-descriptor matrix X;

(b) representing each compound as a column of the molecule-descriptor matrix, the entries of the molecule-descriptor matrix comprising a mathematical function of the weighting of each descriptor for each compound;

(c) performing a partial singular value decomposition (SVD) of the molecule-descriptor matrix to produce resultant matrices P_k, Σ_k, and Q_k, such that partial matrix $X_k = P_k \Sigma_k Q^T{}_k$, is the least squares closest approximation of X for any given k, $k < r$, where r is the rank of the matrix X;

(d) creating a chemical probe descriptor vector, F_1, for the at least one chemical probe, the entries of the chemical probe descriptor vector comprising a mathematical function of the weighting of each descriptor for each chemical probe;

(e) creating a pseudo-object O_{F1}, where $O_{F1} = F_1{}^T P_k \Sigma^{-1}{}_k$;

(f) calculating the similarity between O_{F1} and at least one chemical descriptor i by computing the dot product between row i of matrix P_k and O_{F1}; and

(g) providing an output indicating the similarity between the chemical probe and the at least one chemical descriptor.

27. (New). A method for calculating the similarity of at least one chemical probe, F_1, and at least one other chemical probe, F_2, comprising the steps of:

(a) utilizing at least one chemical descriptor for each of a plurality of compounds, each descriptor comprising a row of a molecule-descriptor matrix X;

(b) representing each compound as a column of the molecule-descriptor matrix, the entries of the molecule-descriptor matrix comprising a mathematical function of the weighting of each descriptor for each compound;

(c) performing a partial singular value decomposition (SVD) of the molecule-descriptor matrix to produce resultant matrices P_k, Σ_k, and Q_k, such that partial matrix $X_k = P_k \Sigma_k Q^T{}_k$, is the least squares closest approximation of X for any given k, $k < r$, where r is the rank of the matrix X;

(d) creating a chemical probe descriptor vector for at least one chemical probe, F_1, the entries of the chemical probe descriptor vector comprising a mathematical function of the weighting of each descriptor for each chemical probe;

(e) creating a pseudo-object O_{F1}, where $O_{F1} = F_1{}^T P_k \Sigma^{-1}{}_k$;

(f) creating a pseudo-object O_{F2}, where $O_{F2} = F_2{}^T P_k \Sigma^{-1}{}_k$;

(g) calculating the similarity between the chemical probe descriptor vector F_1 and the other chemical descriptor probe F_2 by computing the dot product between O_{F1} and O_{F2}; and

(h) providing an output indicating the similarity between the chemical probe, F_1, and chemical probe, F_2.

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28. (New). A method for calculating the similarity of at least one chemical compound to at least one chemical probe, comprising the steps of:

(a) creating at least one descriptor for each compound in a text source;

(b) representing each compound in the text source as at least one mathematical function of the weighting of each descriptor for each compound;

(c) creating a chemical probe descriptor for the at least one chemical probe, the entries of the chemical probe descriptor comprising a mathematical function of the weighting of each descriptor for each chemical probe;

(d) using the text source and the chemical probe descriptor for the at least one chemical probe to calculate a mathematical similarity between the text source and the chemical descriptor for the at least one chemical probe; and

(e) providing an output indicating the similarity between the at least one chemical probe and the at least one chemical compound.

29. The method as recited in claim 2, wherein each of the at least one chemical descriptors further comprise at least one of a charge pair descriptor, a hydrophobic pair descriptor, an inherent atom property descriptor, and a geometry descriptor.